D-Alanine, N-(2-chlorobenzoyl)-, undecyl ester

Inchi: InChI=1S/C21H32ClNO3/c1-3-4-5-6-7-8-9-10-13-16-26-21(25)17(2)23-20(24)18-14-11-1
InchiKey: KPYZULNKYBAKJC-UHFFFAOYSA-N
Formula: C21H32ClNO3
SMILES: CCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 381.94

Physical Properties

Property code	Value	Unit	Source
gf	-59.10	kJ/mol	Joback Method
hf	-576.64	kJ/mol	Joback Method
hfus	53.96	kJ/mol	Joback Method
hvap	91.61	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.532		Crippen Method
mcvol	314.220	ml/mol	McGowan Method
pc	1253.03	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	928.86	K	Joback Method
tc	1141.37	K	Joback Method
tf	555.04	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.51	J/mol×K	928.86	Joback Method
cpg	1009.49	J/mol×K	964.28	Joback Method
cpg	1023.30	J/mol×K	999.70	Joback Method
cpg	1035.97	J/mol×K	1035.11	Joback Method
cpg	1047.56	J/mol×K	1070.53	Joback Method
cpg	1058.12	J/mol×K	1105.95	Joback Method
cpg	1067.70	J/mol×K	1141.37	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354078&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume